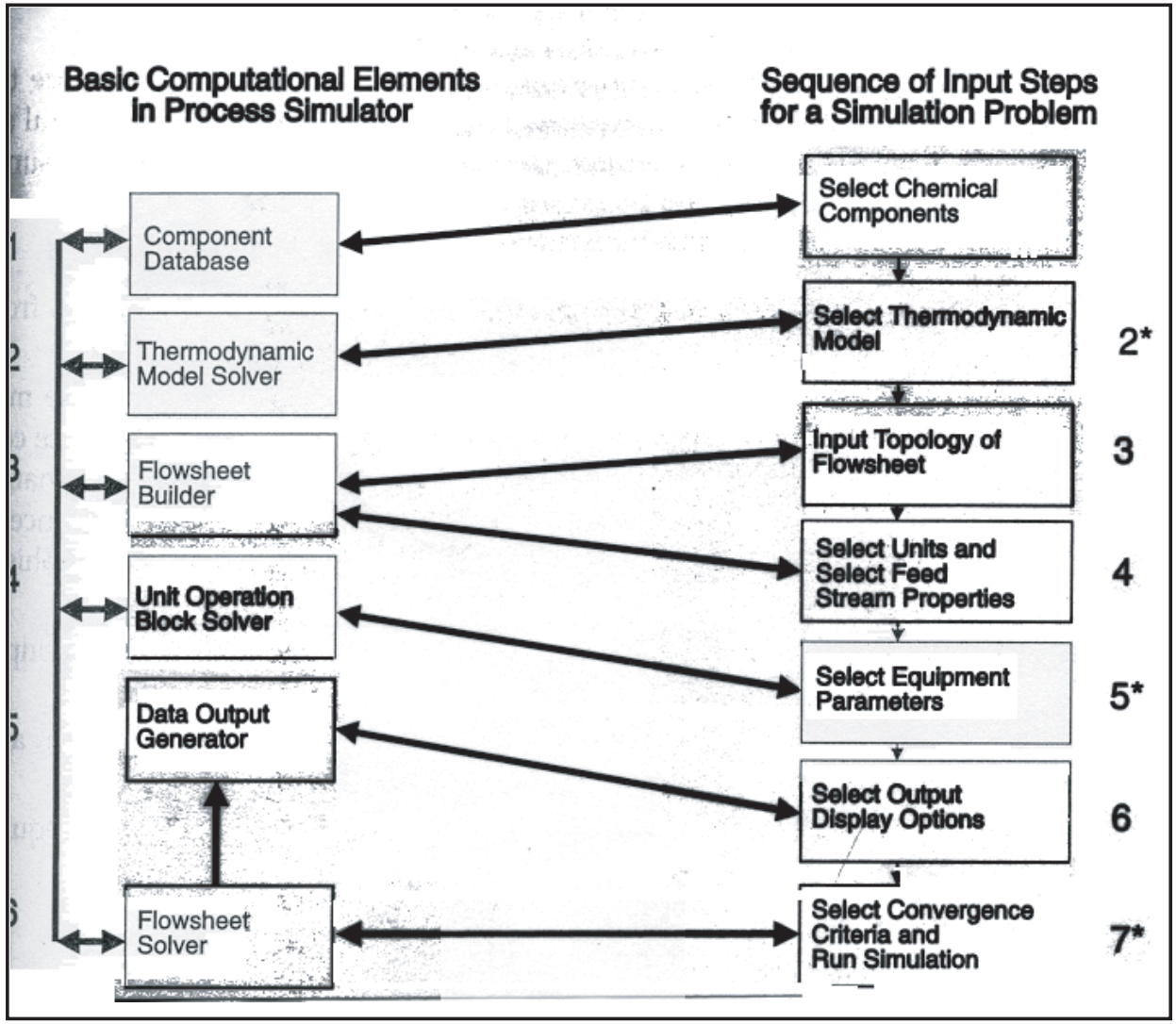
Process Simulators

Using a Process Simulator

Several process simulators are available that facilitate process calculations

- ASPEN PLUS
- HYSIM (now part of ASPEN)
- CHEMCAD
- PRO/II

Simulator Design



Structure of Process Simulator

- Component Database
- Thermodynamic Model Solver
- Flowsheet Builder
- Unit Operation Block Solver
- Data Output Generator
- Flowsheet Solver

General Sequence of Events

- Select topology of flowsheet
- Select chemical components
- Select thermodynamic models
- Select properties of feed streams (temperature, pressure, flowrate, vapor fraction, and composition)
- Select equipment specifications
- Select the way in which the results are to be displayed
- Select the convergence method and run simulation

In general 3, 5, and 7 cause the most problems.

Selecting Thermodynamic Models

- Solution of material and energy balance depends on accurate thermodynamic data.
- Unfortunately, process simulators have default thermodynamics, which will blindly miscalculate the entire flowsheet.
- If the thermodynamic option used by the process simulator is a mystery, the results may be equally mysterious.

Selecting Equipment Parameters

- When first simulating a process, input only the data required to perform the material and energy balance for the process.
- Add complexity in steps.

Selecting Convergence Method

If the simulation has not converged, the results do not represent a valid solution and should not be used.
When convergence is not achieved, the causes could be:

- The problem is ill-posed.
- The tolerance for the solution has been set too tightly.
- The number of iterations is not sufficient.

Please read Chapter 11 from TBWS for more details.